

Superfluidity and magnetism in multicomponent ultracold fermions

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We study the interplay between superfluidity and magnetism in a multicomponent gas of ultracold fermions. Ward-Takahashi identities constrain possible mean-field states describing order parameters for both pairing and magnetization. The structure of global phase diagrams arises from competition among these states as functions of anisotropies in chemical potential, density, or interactions. They exhibit first and second order phase transition as well as multicritical points, metastability regions, and phase separation. We comment on experimental signatures in ultracold atoms.

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Fermionic s -wave superfluidity requires pairing between fermions with different internal states. However, the nature of superfluidity for $N = 2$ component systems and $N \geq 3$ is fundamentally different. Superfluidity *is suppressed by* magnetization for $N = 2$ because there is one way to pair and not every particle can find a partner. This led to proposals for exotic paired states with broken translational symmetry [1, 2] or gapless excitations [3, 4]. In contrast, superfluidity *drives* magnetization for $N \geq 3$. Here condensation energy favors enhancing the population for paired components to different degrees depending on the density of states and interaction energy. This occurs by cannibalizing the populations for unpaired components.

Ultracold atoms offer direct access to multicomponent fermionic superfluids. Observation of two component, equal population superfluids used Feshbach resonances to tune interactions [5, 6, 7, 8]. The population for each component is both tunable and essentially conserved, enabling later experiments on superfluidity with imbalance [9, 10]. Recently, scattering lengths and locations of overlapping Feshbach resonances between all three of the nearly degenerate lowest sublevels of ^6Li were measured [11]. This suggests experiments with $N \geq 3$ are within reach.

In this Letter, we consider the interplay of superfluidity and magnetism within a mean-field theory of $N \geq 3$ multicomponent fermions, each individually conserved. We derive a Ward-Takahashi (WT) identity (Eq. 7) which provides fundamental constraints on possible mean-field states describing both pairing Δ and magnetization M . We demonstrate this WT identity naturally leads to a specific form for the microscopic pairing wavefunction which we call diagonal pairing states (DPS) illustrated in Fig. 1. In these states, gapless excitations always exist for N odd and are still possible for N even.

Having classified the mean-field states, we derive global phase diagrams describing the competition among the DPS as shown in Figs. 2 and 3. We focus on phase diagrams tuned by anisotropies in chemical potential or density but the structure is the same for anisotropies in

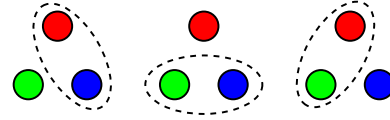


FIG. 1: (color online) Pairing (ellipses) two components (colors) in all possible ways generates the diagonal pairing states as shown for $N = 3$. Only these states generically satisfy the constraints on the microscopic pairing wavefunction imposed by Ward-Takahashi identities derived in the text, linear combinations do not. Paired (unpaired) components have gapped (gapless) quasiparticle excitations.

interactions. For $N \geq 3$, $\Delta\Delta^\dagger$ acts as an external field for M through $M\Delta\Delta^\dagger$. This coupling vanishes identically on group theoretical grounds for $N = 2$ where M couples to Δ only at higher order. The structure of the DPS shows pairing *always* drives magnetization for N odd and *generically* does so for N even through the coupling $M\Delta\Delta^\dagger$. First order transitions and corresponding metastability as well as phase separation regions separate different DPS while second order transitions separate DPS and the normal state. These transitions terminate at bicritical and multicritical points.

Previous theoretical works have also addressed superfluidity with $N \geq 3$ components of fermions. This includes analysis of mean-field states for $N = 3$ [12, 13] and $N = 4$ [14] as well as phase diagrams for $N = 3$ [15, 16]. We focus on classification of allowed pairing states through general symmetry arguments and Ward-Takahashi identities. This complementary approach allows us to obtain generic and robust features of both the resulting states and phase diagrams as well as providing a unified perspective on pairing in multicomponent fermionic systems.

We consider the action $S(H) = S_0 + S_{int}(\Gamma)$ where

$$S_0(H) = \sum_{\alpha\beta} \left[\left(\partial_\tau + \frac{\nabla^2}{2m} \right) \delta_{\alpha\beta} - H_{\alpha\beta} \right] \bar{\psi}_\alpha \psi_\beta, \quad (1)$$

$$S_{int}(\Gamma) = - \sum_{\alpha\beta\gamma\delta} \Gamma_{\alpha\beta\gamma\delta} \bar{\psi}_\alpha \bar{\psi}_\beta \psi_\gamma \psi_\delta$$

describing a dilute gas of fermions with mass m and attractive contact interactions where $\psi_\alpha, \bar{\psi}_\alpha$ with $\alpha = 1 \dots N$ are Grassman variables. The partition function is $Z(H, \Gamma) = \int \mathcal{D}[\bar{\psi}, \psi] \exp \left[- \int_0^\beta d\tau \int d^D \mathbf{x} S(H, \Gamma) \right]$, β is the inverse temperature, D the dimensionality, and $k_B = \hbar = 1$.

We consider general H and Γ to derive WT identities, but the physical system with individually conserved components has $H_{\alpha\beta} = \mu_\alpha \delta_{\alpha\beta}$, $\Gamma_{\alpha\beta\gamma\delta} = \frac{1}{4}(\lambda_{\alpha\gamma} + \lambda_{\beta\delta})\delta_{\alpha\delta}\delta_{\beta\gamma} - (\gamma \leftrightarrow \delta)$ contributing $\mu_\alpha n_\alpha$ and $\lambda_{\alpha\beta} n_\alpha n_\beta$ to the action where $n_\alpha = \bar{\psi}_\alpha \psi_\alpha$. Here μ_α is a chemical potential while $\lambda_{\alpha\beta}$ describes interactions between fermionic densities.

The action is $U(N)$ symmetric for $\mu_\alpha = \mu$ and $\lambda_{\alpha\beta} = \lambda$. This group acts as

$$\psi_\alpha \rightarrow \psi'_\alpha = \sum_\beta U_{\alpha\beta} \psi_\beta, \quad \bar{\psi}_\alpha \rightarrow \bar{\psi}'_\alpha = \sum_\beta \bar{\psi}_\beta U_{\beta\alpha}^\dagger \quad (2)$$

with $U_{\alpha\beta}$ a unitary matrix. Anisotropies in μ_α and $\lambda_{\alpha\beta}$ explicitly break $U(N) \rightarrow U(1)^N$ describing N conserved densities in the normal state. The superfluid state spontaneously breaks $U(N) \rightarrow U(1)^N \rightarrow U(1)^{N-P}$ where P is the number of non-zero pairing amplitudes.

When Eq. 2 is viewed as a field redefinition transformation, the coupling constants also transform $H_{\alpha\beta} \rightarrow H'_{\alpha\beta} = \sum_\gamma U_{\alpha\gamma} H_{\gamma\delta} U_{\delta\beta}^\dagger$, $\Gamma_{\alpha\beta\gamma\delta} \rightarrow \Gamma'_{\alpha\beta\gamma\delta} = \sum_{\mu\nu\rho\sigma} U_{\alpha\mu} U_{\beta\nu} \Gamma_{\mu\nu\rho\sigma} U_{\rho\gamma}^\dagger U_{\sigma\delta}^\dagger$ in order to describe the same physical system. By definition, $Z(H, \Gamma) = Z(H', \Gamma')$ is invariant.

This invariance arises from a field redefinition and is not a physical symmetry. However, it still gives a WT identity (see Ref. [18]) expressing $Z(H, \Gamma) = Z(H', \Gamma')$ under an infinitesimal transformation to first order

$$(\mu_\alpha - \mu_\beta) \frac{\delta Z(H, \Gamma)}{\delta H_{\beta\alpha}} + \sum_\gamma (\lambda_{\alpha\gamma} - \lambda_{\gamma\beta}) \frac{\delta Z(H, \Gamma)}{\delta \Gamma_{\gamma\beta\alpha\gamma}} = 0 \quad (3)$$

for arbitrary α, β . Equivalently, the above equation constrains the expectation value of a redundant operator [19] associated with the field redefinition of Eq. 2 to be zero. This constraint is most useful in the presence of anisotropies and is trivially satisfied in the symmetric limit. Analyzing infinitesimal transformations to second order may yield information about the symmetric limit. We classify possible mean-field states by analyzing the above constraint within the saddle-point approximation discussed next.

Introducing bosonic pairing $\Delta_{\alpha\beta}$ and magnetization $M_{\alpha\beta}$ fields decouples the fermionic interaction through a Hubbard-Stratonovich transformation [17]. Mean-field states are given by zero-momentum, τ -independent expectation values for the order parameters $M_{\alpha\beta}, \Delta_{\alpha\beta}$ satisfying the saddle-point equations

$$M_{\alpha\beta} = T g_M \sum_{\omega_n, \mathbf{k}} G_{\alpha\beta}, \quad \Delta_{\alpha\beta} = \frac{T g_{\Delta, \alpha\beta}}{2} \sum_{\omega_n, \mathbf{k}} F_{\alpha\beta} \quad (4)$$

where $\omega_n = (2n+1)\pi/\beta$ are Matsubara frequencies, \mathbf{k} are momenta, T is the temperature and $\lambda_{\alpha\beta} = \frac{1}{4}g_{\Delta, \alpha\beta} - \frac{1}{2}g_M \left(1 + \frac{1}{N}\right)$ for decoupling interaction anisotropies in the pairing channel. Normal $G_{\alpha\beta}(i\omega_n, \mathbf{k})$ and anomalous $F_{\alpha\beta}(i\omega_n, \mathbf{k})$ Green's functions satisfy

$$\begin{bmatrix} G & F^\dagger \\ F & -G^\dagger \end{bmatrix} = \begin{bmatrix} -\xi - H + M & \Delta^\dagger \\ \Delta & \xi^\dagger + H^\dagger - M^\dagger \end{bmatrix}^{-1} \quad (5)$$

where $\xi_{\alpha\beta} = (i\omega_n - \mathbf{k}^2/2m)\delta_{\alpha\beta}$ in a matrix notation with suppressed indices. As matrices, $M^\dagger = M$ and $H^\dagger = H$ are Hermitian while $\Delta^T = -\Delta$ is skew-symmetric.

Diagonalizing these matrices gives

$$M = \sum_{i=1}^N M_i \mathbf{u}_i \mathbf{u}_i^\dagger, \quad \Delta = \sum_{i=1}^{\lfloor N/2 \rfloor} \Delta_i (\mathbf{v}_{2i-1} \mathbf{v}_{2i}^T - \mathbf{v}_{2i} \mathbf{v}_{2i-1}^T) \quad (6)$$

where $\lfloor x \rfloor$ is the floor function, M_i (Δ_i) real (complex) eigenvalues, and $\mathbf{u}_i^\dagger \mathbf{u}_j = \mathbf{v}_i^\dagger \mathbf{v}_j = \delta_{ij}$ orthonormal eigenvectors. From $M_{\alpha\beta} \sim \langle \psi_\alpha \psi_\beta \rangle$, the physical interpretation of \mathbf{u}_i is the linear combination of fermions giving magnetization M_i . Similarly, $\Delta_{\alpha\beta} \sim \langle \psi_\alpha \psi_\beta \rangle$ shows $\mathbf{v}_{2i-1}, \mathbf{v}_{2i}$ give the two linear combinations of fermions paired with amplitude Δ_i .

From Eq. 3, the WT identity relating M and Δ

$$(\mu_\alpha - \mu_\beta) g_M^{-1} M_{\alpha\beta} + \sum_\gamma \left(g_{\Delta, \alpha\gamma}^{-1} - g_{\Delta, \gamma\beta}^{-1} \right) \Delta_{\alpha\gamma} \Delta_{\gamma\beta}^\dagger = 0 \quad (7)$$

only constrains the off-diagonal elements as a matrix equation. In the normal state $\Delta_{\alpha\beta} = 0$ implying $M_{\alpha\beta} = 0$ for $\alpha \neq \beta$. Physically, $U(1)^N$ symmetry of N conserved densities prohibits mixing between different components.

Superfluidity spontaneously breaks factors of $U(1)$ through off-diagonal elements of $\Delta_{\alpha\beta}$. We now show the WT identity requires the eigenvectors to be of the form

$$\mathbf{u}_{i,\alpha} = \mathbf{v}_{i,\alpha} = S_{i,\alpha} \quad (8)$$

where $S_{i,\alpha}$ is a $N \times N$ permutation matrix with exactly one non-zero matrix element in each row and column. We denote these states the DPS. Consider the generic case when $\mu_\alpha \neq \mu_\beta$, $g_{\Delta, \alpha\beta}^{-1} \neq g_{\Delta, \gamma\delta}^{-1}$. For $N = 3$, the DPS give *all possible mean-field states*. States not of DPS form do not satisfy Eq. 7. For $N > 3$, the DPS give *generic mean-field states*. States not of DPS form can in principle satisfy Eq. 7, but off-diagonal elements are generally overdetermined by the saddle-point equations implying non-zero values are inconsistent.

We now discuss some properties of DPS. They simplify Eq. 4 by decoupling them to $\lfloor N/2 \rfloor$ saddle-point equations each involving only Δ_i, M_{2i-1} , and M_{2i} . M is also diagonal and respects $U(1)^N$ symmetry as in the normal state while Δ breaks P factors of $U(1)$ where P is the number of non-zero Δ_i . The microscopic pairing wavefunction for the DPS is given by using a Bardeen-Cooper-Schrieffer (BCS) s -wave state to pair two and only two

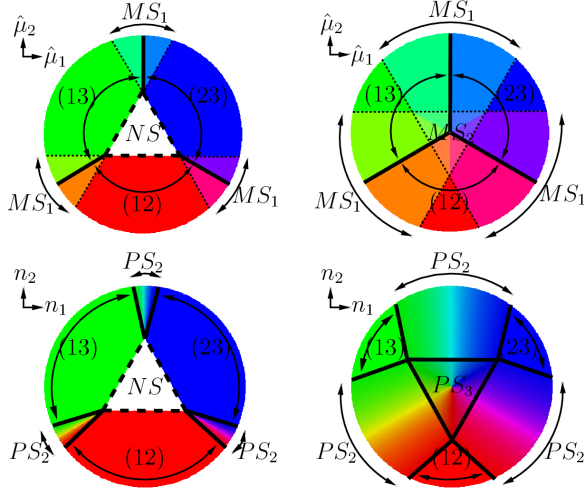


FIG. 2: (color online) $N = 3$ phase diagrams for $T > T_c^{SYM}$ (left) and $T < T_c^{SYM}$ (right) against anisotropies in chemical potential $\hat{\mu}_\alpha$ (top) and density n_α (bottom). NS denotes the normal state and $(\alpha\beta)$ a state with α, β paired. Solid (dashed) lines are first (second) order transitions while dotted lines are boundaries for metastability regions. MS_i denotes regions with i additional metastable paired states and PS_i a phase-separated mixture of i paired states.

components at a time in all possible ways. The WT identity prohibits states given by linear combinations of the DPS. This gives a discrete set of mean-field states with $N!/P!(N-2P)!2^P$ DPS for fixed N and P giving a total of $(i/\sqrt{2})^N H_N(-i/\sqrt{2})$ distinct states for fixed N with $H_n(x)$ the Hermite polynomial.

Quasiparticle excitations are gapped for paired components and are gapless for unpaired components which remain a Fermi liquid. There are at most $\lfloor N/2 \rfloor$ non-zero Δ_i implying one component is always gapless for N odd. For N even, a fully gapped quasiparticle spectrum occurs only when all Δ_i are non-zero. Refs. [12, 13] obtained similar results for $N = 3$.

For simplicity, we construct phase diagrams in the weak-coupling or BCS regime near the superfluid transition for small anisotropies but stress the preceding analysis of the DPS is general. We minimize the free energy

$$\begin{aligned}
 F = & \text{Tr} \left[\frac{1 - 2\hat{g}_M a}{2\hat{g}_M} \delta\hat{M} \delta\hat{M} + b \frac{T - T_c^{SYM}}{T_c^{SYM}} \hat{\Delta}^\dagger \hat{\Delta} \right] + \\
 & \text{Tr} \left[c \delta\hat{M} \hat{\Delta} \hat{\Delta}^\dagger + d \hat{\Delta}^\dagger \hat{\Delta} \hat{\Delta}^\dagger \hat{\Delta} \right] + \sum_\alpha 2a \delta\hat{\mu}_\alpha \delta\hat{M}_{\alpha\alpha} + \\
 & \sum_{\alpha\beta} \left(\delta\hat{g}_{\Delta,\alpha\beta}^{-1} - c \frac{\delta\hat{\mu}_\alpha + \delta\hat{\mu}_\beta}{2} \right) \hat{\Delta}_{\alpha\beta}^\dagger \hat{\Delta}_{\beta\alpha}
 \end{aligned} \quad (9)$$

given by $F = -T \log Z$ where we take $\mu_\alpha = E_F + \delta\mu_\alpha$, $g_{\Delta,\alpha\beta}^{-1} = g_{\Delta}^{-1} + \delta g_{\Delta,\alpha\beta}^{-1}$, $M_{\alpha\beta} = g_M n(E_F) + \delta M_{\alpha\beta}$ with E_F the Fermi energy, $n(E_F)$ the free fermion density and from here on, quantities with a hat are rescaled

with respect to T_c^{SYM} , the critical temperature without anisotropies. Here a, b, c, d are Ginzburg-Landau parameters with $a, b, d \sim \hat{E}_F^{(D-2)/2}$ proportional to the density of states at \hat{E}_F describing particle-hole symmetric contributions. In contrast, $c \sim \hat{E}_F^{(D-4)/2}$ for $D = 2$ and $c \sim \hat{E}_F^{(D-4)/2} \log \hat{E}_F$ for $D \neq 2$ is essentially proportional to the derivative of the density of states at \hat{E}_F and describes particle-hole symmetry breaking contributions.

$U(N)$ symmetric terms are under Tr , the matrix trace. Notice the $\delta\hat{M} \hat{\Delta} \hat{\Delta}^\dagger$ term where $\hat{\Delta} \hat{\Delta}^\dagger$ acts as an external field to $\delta\hat{M}$. On group theoretical grounds, this term is non-vanishing only for $N \geq 3$. Terms outside the trace explicitly break $U(N) \rightarrow U(1)^N$, including a term quadratic in $\hat{\Delta}$. The structure of global phase diagrams follows from these two terms.

Pairing $\hat{\Delta} \hat{\Delta}^\dagger$ drives magnetization $\delta\hat{M}$ unless $\hat{\Delta} \hat{\Delta}^\dagger \propto \mathbf{1}$ is particle-hole symmetric with $\mathbf{1}$ the identity matrix. In this case, a shift in chemical potentials described by \hat{M} yields no gain in condensation energy. Only when all components pair and $|\Delta_i| = |\Delta_j|$ does this occur. For N odd, one component is always unpaired so magnetization always develops. For N even, only when the $N/2$ independent equations determining Δ_i give $|\Delta_i| = |\Delta_j|$ is it possible to have pairing without magnetization.

A similar situation occurs for p -wave pairing in ^3He or the organic superconductors. Unitary states describe pairing decoupled from magnetization while non-unitary states describe pairing coupled to magnetization [20]. Only a single constraint $|\mathbf{d} \times \mathbf{d}^*| = 0$ on the \mathbf{d} -vector describing p -wave pairing is necessary for a unitary state. It is more difficult for the $N/2$ independent equations determining Δ_i to give $|\Delta_i| = |\Delta_j|$ for the analog of unitary states in multicomponent s -wave pairing.

We now discuss the $N = 3$ phase diagram in Fig. 2 with given interactions satisfying the generic condition $\delta\hat{g}_{\Delta,\alpha\beta}^{-1} \neq \delta\hat{g}_{\Delta,\gamma\delta}^{-1}$. We consider both fixed chemical potential $\hat{\mu}_\alpha$ and fixed particle density n_α as

$$\begin{aligned}
 \hat{\mu}_\alpha &= \hat{E}_F \mathbf{x}_{0,\alpha} + \hat{\mu}_1 \mathbf{x}_{1,\alpha} + \hat{\mu}_2 \mathbf{x}_{2,\alpha}, \\
 n_\alpha &= n(E_F) \mathbf{x}_{0,\alpha} + n_1 \mathbf{x}_{1,\alpha} + n_2 \mathbf{x}_{2,\alpha}
 \end{aligned} \quad (10)$$

where $\mathbf{x}_0 = [1, 1, 1]$, $\mathbf{x}_1 = [1, -1, 0]/\sqrt{2}$, $\mathbf{x}_2 = [1, 1, -2]/\sqrt{6}$ and $\hat{\mu}_i, n_i$ parameterize anisotropies.

First consider fixed $\hat{\mu}_\alpha$ (top Fig. 2). When $T > T_c^{SYM}$, small anisotropy favors the normal state. Increasing anisotropy favors pairing by increasing the density of states for some components at the expense of others. This drives a second order transition into one of the three DPS. Tuning the direction of the anisotropy drives first order transitions between DPS when two of these states are degenerate along lines of enhanced symmetry. First order lines terminate at bicritical points from which metastability regions where an additional DPS is locally stable branch out. This is the expected behavior for quadratic symmetry breaking [21, 22]. Bicritical points

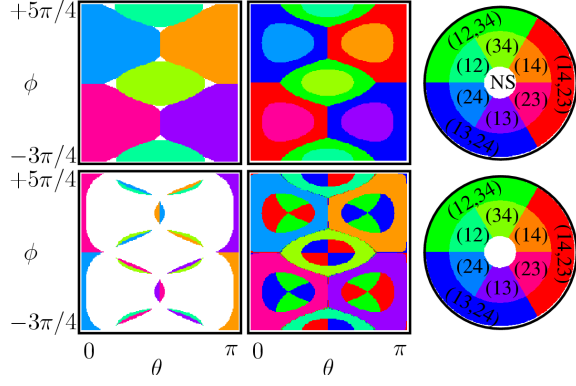


FIG. 3: (color online) Representative $N = 4$ phase diagrams for $T > T_c^{SYM}$ (left) and $T < T_c^{SYM}$ (middle) against 0 in chemical potential μ_α with legend (right) for the global minimum (top) and first metastable state (bottom). $(\alpha_i \beta_i, \dots)$ denotes α_i, β_i paired and white regions NS the normal state (top) or absence of metastable states (bottom). First (second) order transitions separate different paired states (paired states from the normal state).

terminate at the $U(3)$ symmetric multicritical point when $T = T_c^{SYM}$. Below T_c^{SYM} , first order lines separate DPS and a region near small anisotropy where all three DPS are (meta)stable appears.

The Maxwell construction gives fixed n_α phase diagrams (bottom Fig. 2) from those for fixed $\hat{\mu}_\alpha$. The compressibility tensor $\kappa_{\alpha\beta} \propto -\partial^2 F / \partial \hat{\mu}_\alpha \partial \hat{\mu}_\beta$ at fixed $\hat{\mu}_\alpha$ has positive eigenvalues except at boundaries between DPS. Here, $\hat{\Delta} \hat{\Delta}^\dagger$ and thus $\delta \hat{M}$ jump discontinuously. First order lines at fixed $\hat{\mu}_\alpha$ when two DPS are degenerate expand into phase-separated mixtures of those two states at fixed n_α . For $T < T_c^{SYM}$, the zero anisotropy point where all three DPS are degenerate expands into a phase-separated mixture of those three states at fixed n_α .

Now consider the $N = 4$ phase diagram in Fig. 3 with fixed chemical potential given by

$$\begin{aligned} \hat{\mu}_\alpha = & \hat{E}_F \mathbf{y}_{0,\alpha} + \hat{\mu}_0 \cos(\theta) \mathbf{y}_{1,\alpha} + \\ & \hat{\mu}_0 \sin(\theta) \cos(\phi) \mathbf{y}_{2,\alpha} + \hat{\mu}_0 \sin(\theta) \sin(\phi) \mathbf{y}_{3,\alpha} \end{aligned} \quad (11)$$

where $\mathbf{y}_0 = [1, 1, 1, 1]$, $\mathbf{y}_1 = [1, -1, 0, 0]/\sqrt{2}$, $\mathbf{y}_2 = [1, 1, -2, 0]/\sqrt{6}$, $\mathbf{y}_3 = [1, 1, 1, -3]/\sqrt{12}$ and θ, ϕ the anisotropies.

For $N > 3$, condensation energy favors development of more pairing amplitudes as T is lowered. The normal state competes with the six DPS with only one pairing amplitude for $T > T_c^{SYM}$ (top right Fig. 3). However, the three DPS with two pairing amplitudes and all components paired eventually dominate the phase diagram for $T < T_c^{SYM}$ (top middle Fig. 3). Phase diagrams still exhibit second order transitions from the normal state to DPS and first order transitions between DPS.

We now comment on trapping effects and detection methods for applications to ultracold atoms. In the large

particle number BCS regime, the local density approximation accurately maps phase diagrams at fixed chemical potential to phase diagrams with trapping. DPS are distinguished by both densities and pairing amplitudes for different components. State-selective imaging of density distributions [9, 10] and radio-frequency spectroscopy of the pairing gap [23] can be used to detect signatures of the various paired states.

In summary, we have studied the essential role magnetism plays in superfluidity of multicomponent fermions. By analyzing constraints imposed by Ward-Takahashi identities, we classified the allowed mean-field pairing states with both magnetization and pairing order parameters and used them to construct global phase diagrams. These phase diagrams have a rich structure with first and second order transitions meeting at multicritical points as well as metastability and phase separated regions. We discussed applications to ultracold fermions.

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